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Lithium trifluoromethanesulfonate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(O–Li) = 0.003 Å
R factor = 0.029
wR factor = 0.078
Data-to-parameter ratio = 14.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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The title compound, $Li^{+}\cdot CF_3SO_3^{-}$, has already been investigated by powder diffraction methods. We present in this work the single-crystal structure, which is in good agreement with the previous structure determination.

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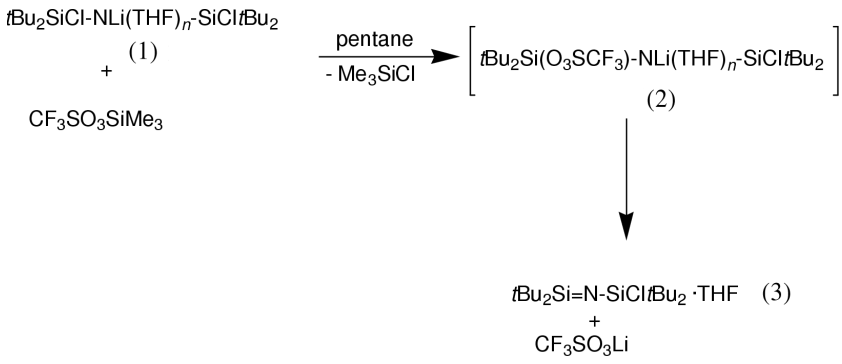
Comment

We have recently shown that silanimine can be generated by CF_3SO_3Li (TfLi) elimination from silylamides, R_2SiTf–NLi–R' (Wiberg & Lerner, 1996; Lerner, 1994). Treatment of silylamide (1) with $CF_3SO_3SiMe_3$ in pentane leads to the displacement of a Cl atom by a CF_3SO_3 unit, to yield the amide (2) and Me_3SiCl. While the trifluoromethanesulfonate anion is a better leaving group than the Cl^{-} anion, the respective compound (2) reacts to the silanimine (3) and CF_3SO_3Li.



The crystal structure of the title compound, (3), compares well with the study carried out employing powder diffraction data (Tremayne *et al.*, 1992). On the other hand, there are some minor differences owing to the different temperatures at which the data sets were collected and the different methods employed: the cell parameters of the structure determined by powder diffraction are a little larger (due to the higher temperature) but their s.u.'s are lower. The s.u.'s of the coordinates, however, are a factor of ten lower in the single-crystal structure. Furthermore, we were able to refine all atoms anisotropically, a benefit of the better data-to-parameter ratio, leading to better determined geometric parameters.

Experimental

$CF_3SO_3SiMe_3$ (0.5 ml, 3.06 mmol) was added with stirring at room temperature to a solution of $^{t}Bu_2SiCl$–NLi(thf)$_n$SiCl$^{t}Bu_2$ (3.04 mmol; Lerner, 1994) in pentane (25 ml). Colourless crystals of the title compound were obtained after 48 h.

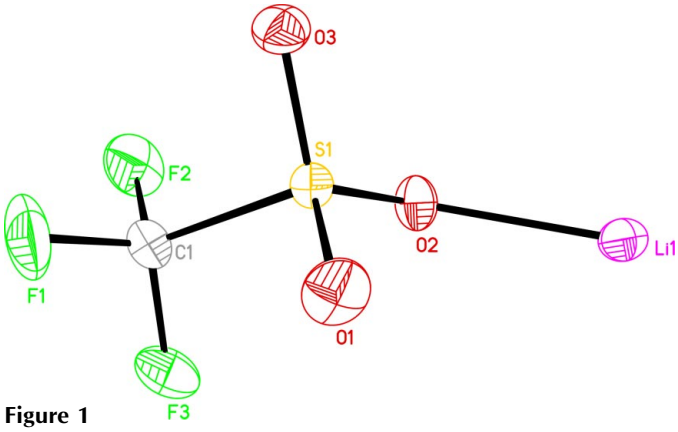


Figure 1
A perspective view of the asymmetric unit of title compound with the atom-numbering scheme. Displacement ellipsoids are at the 50% probability level.

Crystal data

$Li^{+}\cdot CF_3SO_3^{-}$
M_r = 156.01
Monoclinic, $P2_1/c$
a = 10.0994 (6) Å
b = 5.0410 (2) Å
c = 9.5320 (6) Å
β = 90.370 (5)°
V = 485.27 (5) Å^3
Z = 4
D_x = 2.135 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 500 reflections
θ = 4.–20.8°
μ = 0.66 mm^{-1}
T = 173 (2) K
Block, colourless
0.36 × 0.22 × 0.16 mm

Data collection

Siemens CCD three-circle diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.798, T_{max} = 0.902
7664 measured reflections
1144 independent reflections
966 reflections with $I > 2\sigma(I)$
R_{int} = 0.032
θ_{max} = 29.5°
$h = -13 \rightarrow 13$
$k = -6 \rightarrow 6$
$l = -12 \rightarrow 12$
123 standard reflections
frequency: 1200 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.078
S = 1.12
1144 reflections
82 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.2268P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.4351 (13)	C1—F2	1.328 (2)
S1—O3	1.4351 (13)	Li1—O1^{i}	1.873 (3)
S1—O2	1.4500 (13)	Li1—O2	1.995 (3)
S1—C1	1.8212 (18)	Li1—O2^{ii}	1.988 (3)
C1—F1	1.311 (2)	Li1—O3^{iii}	1.901 (3)
C1—F3	1.318 (2)		
O1—S1—O3	115.70 (9)	F1—C1—F3	109.63 (15)
O1—S1—O2	112.67 (8)	F1—C1—F2	108.87 (15)
O3—S1—O2	114.08 (8)	F3—C1—F2	108.73 (17)

Symmetry codes: (i) $2-x, y-\frac{1}{2}, \frac{1}{2}-z$; (ii) $2-x, -y, -z$; (iii) $2-x, 1-y, -z$.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991).

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